

Multidimensional Mesh Approaches to Calculations of Atoms and Diatomic Molecules in Strong Electric Fields

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Abstract. Fully numerical mesh solutions of 2D and 3D quantum equations of Schrödinger and Hartree-Fock type allow us to work with wavefunctions which possess a very flexible geometry. This flexibility is especially important for calculations of atoms and molecules in strong external fields where neither the external field nor the internal interactions can be considered as a perturbation. In the framework of this method we present various approaches to calculations of quasi-steady states of these systems in strong electric fields. These approaches are aimed at obtaining precise complex wavefunctions and corresponding eigenvalues in the form $E = E_0 - i\Gamma/2$, where E_0 is the real part of the energy and the value $\Gamma/2$ determines the lifetime of the state in relation to escape of electrons from the system. The applications for single-electron systems include correct solutions of the Schrödinger equation for the H_2^+ ion (energies and decay rates) and the hydrogen atom in strong parallel electric and magnetic fields. Some results for the helium atom in strong electric fields are announced.

I INTRODUCTION

During the latter decade the interest to theoretical studies of atoms and molecules in strong external fields was strongly motivated by experiments with intense laser beams (electromagnetic fields with dominating electric component) and astronomical observations of white dwarfs and neutron stars (magnetic fields). The experimental availability of extremely strong electric fields in laser beams makes the theoretical study of various atomic and molecular species under such conditions very desirable. The properties of atomic and molecular systems in strong fields undergo dramatic changes in comparison with the field-free case. These changes

are associated with the strong distortions of the spatial distributions of the electronic density and correspondingly the geometry of the electronic wavefunctions. This complex geometry is difficult for its description by means of traditional sets of basis functions and requires more flexible approaches which can, in particular, be provided by multi-dimensional mesh finite-difference methods.

Many results of the experiments with intense laser beams can be considered from the point of view of the behaviour of atoms and molecules in intense static electric fields, especially when the frequency of the radiation is low. (The low-frequency behaviour and the limits of this region are analysed by [1]).

The most advanced theoretical studies of effects in strong electric fields were traditionally concentrated on a hydrogen atom. Other atomic and molecular systems in strong electric fields are much less studied. Many sophisticated theoretical methods developed for the hydrogen atom cannot be simply applied for other atoms and molecules. This circumstance is an argument for development of more universal theoretical and computational methods for atoms and molecules in strong electric fields.

Quasi-steady states of hydrogen atoms in strong electric fields were studied precisely in many theoretical works (see [2–11] and references therein). Some of these works are based on separation of variables in parabolic coordinates in the Schrödinger equation for the hydrogen atom. This separation of spatial variables for atomic and molecular systems in external electric fields is possible only for one-electron atoms with the Coulomb electron-nucleus interaction. Non-hydrogenic systems or systems with non-Coulomb interaction do not allow this separation of variables. Their theoretical studies require a developed technique of solving the Schrödinger and similar equations with non-separable variables. One of the possible ways for solution of this problem consists in the application of mesh computational methods for solving these equations. The mathematical problem consists here in solution of partial differential equations for systems with discrete quasi-steady states lying on the background of the continuous spectrum.

In the first part of this work we present applications of our mesh method for solving Schrödinger equations with non-separable variables for quasi-steady states. The method is based on the technique of a mesh numerical solution of Schrödinger and Hartree-Fock equations with non-separable variables for steady states [12–17]. The most of the applications for the discrete states was focused on atoms in strong magnetic fields [14–20]. In this paper we present computational approaches which we have developed for quasi-steady states in external electric fields [21–23] and apply them to several single electron systems. At the end of the paper we announce some of results of our current work on the helium atom in strong electric fields.

II FORMULATION OF THE PROBLEM AND THE 2D MESH COMPUTATIONAL METHOD FOR STATIONARY STATES

We carry out our mesh solution in the cylindrical coordinate system (ρ, ϕ, z) with the z -axis oriented along the electric field. After separation of the ϕ coordinate the Hamiltonians of the single-electron problems considered below take the form

$$H = -\frac{1}{2} \left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{\partial^2}{\partial z^2} - \frac{m^2}{\rho^2} \right) + s_z \gamma + \frac{m}{2} \gamma + \frac{\gamma^2}{8} \rho^2 - \frac{1}{r} - Fz \quad (1)$$

– the hydrogen atom in parallel electric and magnetic fields and

$$H = -\frac{1}{2} \left(\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{\partial^2}{\partial z^2} - \frac{m^2}{\rho^2} \right) + s_z \gamma + \frac{m}{2} \gamma + \frac{\gamma^2}{8} \rho^2 - \frac{1}{[(z + R/2)^2 + \rho^2]^{1/2}} - \frac{1}{[(z - R/2)^2 + \rho^2]^{1/2}} - Fz \quad (2)$$

– the molecular ion H_2^+ in electric and magnetic fields parallel to the molecular axis. Here and in the following the atomic units $m_e = \hbar = e = 1$ will be used, including the magnetic field strength γ measured in units $B_0 = \hbar c / e a_0^2 = 2.3505 \cdot 10^5 \text{T}$, $\gamma = B/B_0$. F is the electric field strength multiplied by the charge of the electron. $F = 1$ corresponds to 51.422V/\AA . The value m is the magnetic quantum number and $s_z = \pm \frac{1}{2}$ is the spin z -projection. R is the internuclear distance for H_2^+ molecule. The Hamiltonian (2) does not include the internuclear repulsion and its eigenvalues are the electronic energies E_e which are connected with the total energy of H_2^+ by the formula $E = E_e + 1/R$.

Our two-dimensional mesh computational method which we apply for obtaining eigenvalues of the Hamiltonians (1) and (2) in the form sufficient for case of stationary states (i.e $F = 0$) of single-electron systems is described in refs. [13,14]. For these systems highly precisely solutions can be obtained by solving Schrödinger equations in finite spatial domains Ω (with simple boundary conditions $\psi|_{\partial\Omega} = 0$ or $\partial\psi/\partial n|_{\partial\Omega} = 0$) with negligible errors for domains of reasonable dimensions (see analytical estimations of errors in ref. [14] and results of numerical experiments in ref. [13]). When employing the Richardson's extrapolation of the energy values to the infinitely small mesh step $h \rightarrow 0$ very precise results can be obtained on uniform meshes with relatively small numbers of nodes [13,14]. Two important problems have been solved for the following development of the multi-dimensional Hartree-Fock method for many-electron systems: 1. An enhancement of the precision of single-electron wavefunctions due to their more complicated geometry in comparison with the one-electron case, and 2. Obtaining correct mesh representations of Coulomb and exchange potentials. The first of these problems can be solved more or less simply by means of non-uniform meshes with the distribution of

nodes concentrated near the nuclei. The second and most complicated problem was initially solved in our first works on the helium atom in magnetic fields [15,16] by means of a direct summation over the mesh nodes. But this direct method is very expensive with respect to the computing time and due to this reason we obtained in the following works [17–20] these potentials as solutions of the corresponding Poisson equations. The problem of the boundary conditions for a Poisson equation as well as the problem of simultaneously solving Poisson equations on the same meshes with Schrödinger-like equations for the wave functions $\psi_\mu(z, \rho)$ has been discussed in ref. [16].

The simultaneous solution of the Poisson equations for the Coulomb and exchange potentials and the Schrödinger-like equations for the wave functions $\psi_\mu(z, \rho)$ is a complicated problem due to a different asymptotic behaviour of the wavefunctions and potentials. The wavefunctions of the bound electrons decrease exponentially as $r \rightarrow \infty$ (r is the distance from the origin). This simplifies the problem of the solution of equations for wavefunctions in the infinite space because it is possible either to solve these equations in a finite domain Ω (as described above) or otherwise to solve these equations in the infinite space on meshes with exponentially growing distances between nodes as $r \rightarrow \infty$. On the contrary, solutions of Poisson equations for non-zero sums of charges decrease as $1/r$ as $r \rightarrow \infty$. In result, every spatial restriction of the domain Ω introduces a significant error into the final solution. In our approach we address the above problems by using special forms of non-uniform meshes [17]. Solutions to the Poisson equation on separate meshes contain some errors δ_P associated with an inaccurate description of the potential far from the nucleus. However, due to the special form of the function $\delta_P(\tilde{h})$ for these meshes (where \tilde{h} is a formal mesh step) the errors do not show up in the final results for the energy and other physical quantities, which we obtain by means of the Richardson extrapolation procedure (polynomial extrapolation to $h = 0$ [13,14]). The main requirement for these meshes is a polynomial increase of the actual mesh step $h(r)$ when $r \rightarrow \infty$. Moreover, this behaviour can be only linear one, i.e. $h^{-1}(r) = O(1/r)$ as $r \rightarrow \infty$. The error of the mesh solution in this case has the form of a polynomial of the formal step of the mesh $\tilde{h} = 1/N$, where N is the number of nodes along one of the coordinates. In practical calculations these meshes are introduced by means of an orthogonal coordinate transformation from the physical coordinates x_p to the mathematical ones x_m made separately for ρ and z . The numerical solution is, in fact, carried out on uniform meshes in the mathematical coordinates x_m . The characteristic feature of these meshes consists of rapidly increasing coordinates of several outermost nodes when increasing the total number of nodes and decreasing the actual mesh step in the vicinity of the origin.

The methods described above for the two-dimensional case can be applied also to three-dimensional Schrödinger and Hartree-Fock problems [24,25].

III QUASISTATIONARY STATES

The most common approach to the mathematical description of the quasistationary states of quantum systems consists in employment of the complex form of the energy eigenvalues

$$E = E_0 - i\Gamma/2$$

where the real part of the energy E_0 is the centre of the band corresponding to a quasistationary state and the imaginary part $\Gamma/2$ is the half-width of the band which determines the lifetime of the state. In this approach one may consider quasistationary states of quantum systems similarly to the stationary ones. For systems (1) and (2) at $F > 0$ the electron can leave the system in the direction of positive z and the behaviour of the wavefunction on this semi-axis determines the main features of the behaviour in the external electric field F . The mathematical problem consists in the solution of the Schrödinger equation

$$H\psi = E\psi \quad (3)$$

at $F > 0$ for resonance states which are inheritors of some discrete (at $F = 0$) states. The wavefunctions of these states must describe the process of separation of the electron from the system. These wavefunctions can be distinguished either by the explicit establishing the boundary condition of the outgoing wave or by means of a complex coordinate transformation. The latter transforms the oscillating outgoing wave into an exponentially decreasing wavefunction for which the simple Dirichlet boundary condition $\psi \rightarrow 0$ as $z \rightarrow +\infty$ can be established.

From the mathematical point of view the problem under consideration consists in obtaining solutions of the single-particle Schrödinger equation for this electron with

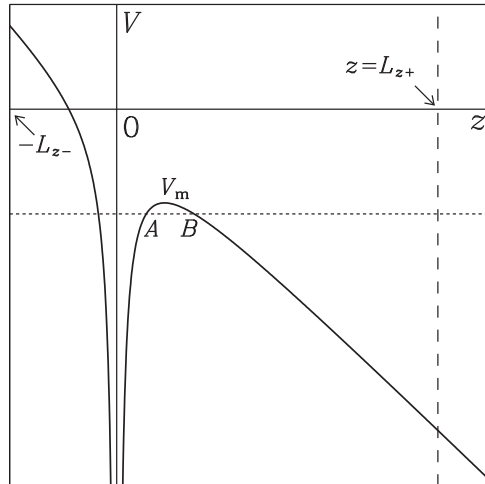


FIGURE 1. The potential energy for the hydrogen atom $V(\rho = 0, z)$ in the external uniform electric field.

the correct asymptotic behaviour of the wavefunction as an outgoing wave. Currently we have three different possibilities for obtaining solutions with the outgoing wave asymptotics realised in our computational program:

1. *Complex boundary condition method.* This method is described in detail in ref. [16,22]. The method is based on the idea that the single-electron Schrödinger equation for a finite system can be solved with the arbitrary precision in a finite area both for stationary and for quasi-stationary eigenstates. The case of stationary states is considered in [13,14]. We discuss the approach for the quasi-stationary states following ref. [22]. Figure 1 presents the potential curve for the simplest Hamiltonian (1). Analogously to [14,27] the calculations can be carried out in an area Ω which is finite along the direction z . For the coordinate z we have used uniform meshes. The boundary of the area $z = -L_{z-}$ for $z < 0$ ($F \geq 0$) (Figure 1) is determined from the condition of small values of the wavefunction on the boundary and, therefore, small perturbations introduced by the corresponding boundary condition [14]. The values of the wavefunction on the opposite boundary of the area ($z = L_{z+}$) cannot be excluded from the consideration. We consider non-stationary states corresponding to the process when an electron leaves the system in the direction $z \rightarrow +\infty$. Thus, an outgoing wave boundary condition is to be established on $z = L_{z+}$. The form of this boundary condition can be derived from the asymptotic behaviour of the wavefunction for $z \rightarrow +\infty$. In this limit the asymptotics of the real system can be replaced by the asymptotics of the wavefunction of a free electron in the uniform electric field. Solutions of the Schrödinger equation for this system can be written as

$$\psi(z) = AM(\xi)e^{-i\Theta(\xi)}, \quad \xi = \left(z + \frac{E}{F}\right)(2F)^{1/3} \quad (4)$$

where $M(\xi)$ and $\Theta(\xi)$ are the modulus and phase of the Airy function, A is a constant [26]. The asymptotics of ψ for $z \rightarrow +\infty$ can be obtained from eqs. (10.4.78) and (10.4.79) of [26] in the form

$$\psi(z) = \frac{A}{\sqrt{\pi}}\xi^{-1/4} \exp\left(-i\frac{\pi}{4} + i\frac{2}{3}\xi^{3/2}\right) + O\left(\xi^{-13/4}\right) \quad (5)$$

Taking into account that $d\xi/dz = (2F)^{1/3}$ and $\xi^{1/2}(2F)^{1/3} = [2(E + Fz)]^{1/2}$ we have from (5)

$$\frac{d\psi}{dz} = \left(ik - \frac{F}{2k^2}\right)\psi + \frac{d}{d\xi}O(\xi^{-13/4}) \quad (6)$$

where $k = [2(E + Fz)]^{1/2}$ is the wavenumber. Equation (6) allows us to establish the following outgoing wave boundary condition on the upper (in the z direction) edge of the region

$$\left.\frac{\partial\psi}{\partial z} + \left(\frac{F}{2k^2} - ik\right)\psi\right|_{z=L_{z+}} = 0 \quad (7)$$

This approximate boundary condition is derived from the asymptotics of the wavefunction of a free electron in a uniform electric field and in the limit $L_{z+} \rightarrow +\infty$ can be considered as exact one. On the other hand, our numerical experiments show, that errors caused by the approximate nature of this asymptotics are important only for very short regions Ω . Solving the Schrödinger equation with the boundary condition (7) established on a reasonable distances L_{z+} from the origin of the system one obtains precise complex eigenvalues of the energy and corresponding wavefunctions.

This straightforward approach enables obtaining precise results both for atoms and molecules from weak to moderate strong fields (for instance for the ground state of the hydrogen atom up to $F = 0.20 - 0.25$ a.u.). For stronger fields the precision of this method is limited by the precision of the mesh representation of the boundary condition (7).

2. *Classical complex rotation of the coordinate z in the form $z \rightarrow ze^{i\Theta}$.* Opposite to the boundary condition approach, this method does not require establishing boundary conditions dependent on the energy and can be used with the zero boundary conditions for the wavefunction. This simplification is especially important for applications to multi-electron systems. In this approach we have obtained precise results for atomic systems in strong fields from the lower bound of the over-barrier regime up to super-strong fields corresponding to regime $|\text{Re}E| \ll |\text{Im}E|$ [23]. For atoms in weak fields the applicability of the method is limited by numerical errors in the imaginary part of the energy. On the other hand, this method cannot be immediately applied to molecular systems in our direct mesh approach [23,28].

3. *Exterior complex transformation of the coordinate z .* The exterior complex scaling [28] combines many advantages of the boundary condition and complex

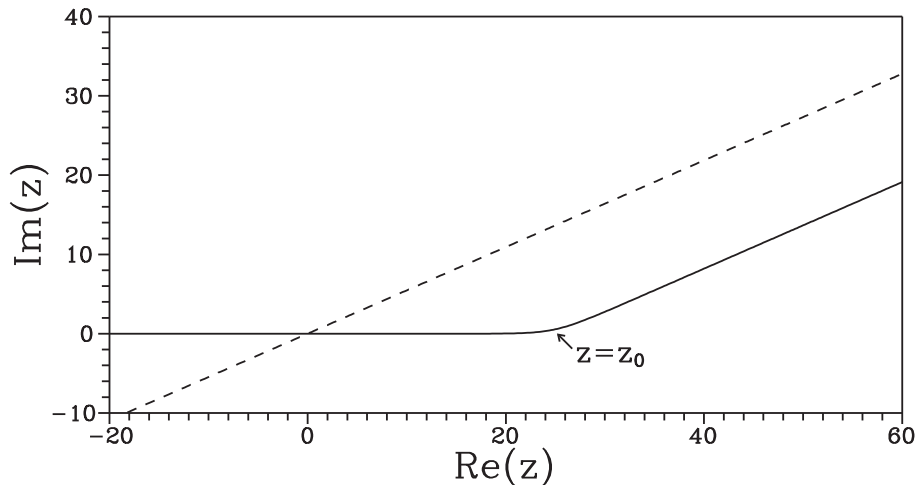


FIGURE 2. The integration paths for the complex coordinate z . Dashed line is the path at the traditional rotation $z \rightarrow ze^{i\Omega}$. Solid line is the path corresponded to the exterior curved path coordinate transformation.

rotation method. In its initial form [28] it consists in the complex rotation of a coordinate e.g. r around a point r_0 lying in the exterior part of the system, i.e.

$$r \rightarrow r_0 + (r - r_0)e^{i\Theta} \quad \text{for } r \geq r_0 \quad (8)$$

and leaves intact the Hamiltonian in the internal part of the system. The latter circumstance allows us to employ this transformation both for atoms and molecules in arbitrary electric fields. In addition this transformation does not contain energy-dependent boundary conditions as well as the classical complex rotation. On the other hand, the exterior complex scaling being introduced into our numerical scheme in the form (8) leads to the same numerical problems at very strong fields as well as the boundary condition method due to the nonanalytic behaviour of this transformation at the point r_0 (or z_0 in our case).

In our numerical approach we solve the latter problem by means of a transformation of the real coordinate z into a smooth curved path in the complex plane z (Figure 2, see details in [23]). This transformation leaves intact the Hamiltonian in the internal part of the system, but supplies the complex rotation of z (and the possibility to use the zero asymptotic boundary conditions for the wavefunction) in the external part of the system without any loss of analyticity. The transformation can be applied both for atoms and molecules and provides precise results for fields from weak up to super-strong including the regime $|\text{Re}E| \ll |\text{Im}E|$ [23].

The three methods presented above have different but overlapping regions of their most effective application. This allows their combined using for the reciprocal control in applications. The numerical results obtained by all three methods coincide in the limits of their applicability and are in agreement with numerous published data on the hydrogen atom in electric fields (see e.g. [5–8]).

IV SELECTED PHYSICAL RESULTS

Using the boundary condition approach enables one to obtain both the values of the energy and other observables and the wavefunctions in their mesh representation. An example of such a wavefunction of the ground state of the hydrogen molecular ion is presented in Figure 3. The electron energy E_e obtained as a solution of (3), (2) allows one to determine potential curves $E(R)$ for the molecule as a whole by using the formula $E(R) = E_e + 1/R$. These potential curves and corresponding values of $\Gamma/2$ are presented in Figure 4. One can see in Figure 4 that when growing electric field strength the minimum on the curve $E(R)$ shifts to the right, becomes more shallow and flat, and at $F_c \approx 0.065$ the minimum disappears. The dependence of the location R_0 of the minimum on these curves with corresponding values of the energy E and half-widths of the level are presented in Table 1. (For comparison, at $F = 0$ published results for the equilibrium point are $R_0 = 1.997193$ and $E = -0.6026346$ [29]. For the potential curve as a whole our numerical values at $F = 0$ coincide with data by [30].) One can see in Table 1

and Figure 4 that for the ground state of the hydrogen molecular ion at equilibrium internuclear distances there is a marked probability of its decay through the separation of the electron. Analogous calculations for two excited states $2p\pi_u$ (the lowest state with $|m| = 1$) and $3d\delta_g$ (the lowest state with $|m| = 2$) [22] show that for the field strengths at which their potential curves have minima this process has a low probability.

The critical value of the maximal electric field $F_c = 0.065 \text{ a.u.} = 3.3 \text{ V/\AA}$ when the molecule H_2^+ can exist is in a good agreement with experimental results by Bucksbaum *et al* [31]. According this work H_2^+ molecule may exist in laser beam fields with intensity less than 10^{14} W/cm^2 which corresponds to 3 V/\AA , and does not exist in more intensive fields.

Other theoretical explanations of the rupture of H_2^+ molecule in intensive laser

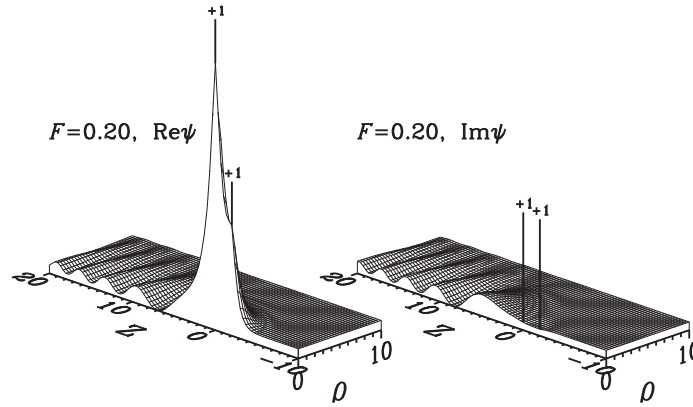


FIGURE 3. Real and imaginary parts of the wavefunction of the H_2^+ molecule in a longitudinal electric field F (a.u.).

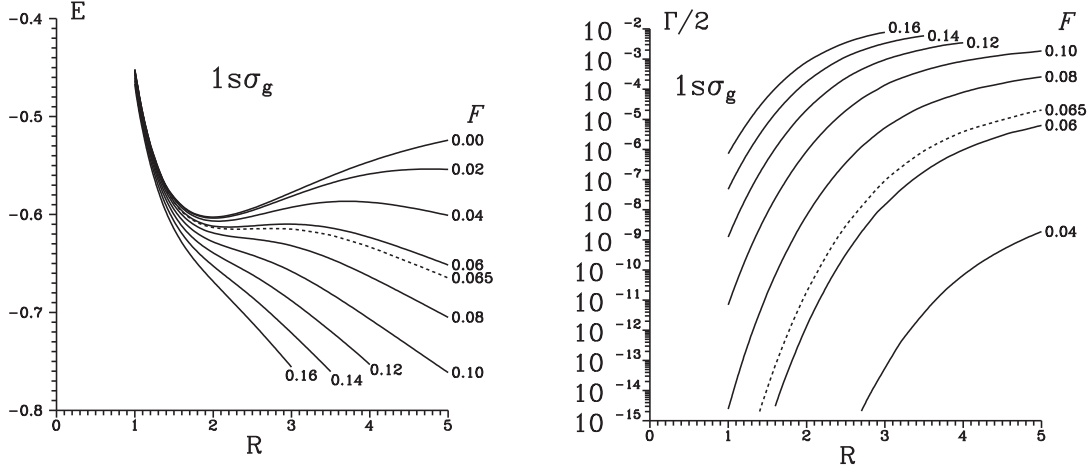


FIGURE 4. Left – Potential curves for the ground state of the H_2^+ molecule in the longitudinal electric field F (a.u.). Right – Half-widths of the ground state energy level of the molecule H_2^+ in the longitudinal electric field F as a function of the internuclear distance R (a.u.).

TABLE 1. Equilibrium internuclear distances and corresponding energies and half-widths of the energy of the ground state of H_2^+ molecule in longitudinal electric fields.

F	R_0	E_0	$\Gamma/2$	F	R_0	E_0	$\Gamma/2$
0.00	1.997	-0.60264	—	0.04	2.062	-0.60686	1.23(-19)
0.01	2.001	-0.60289	—	0.05	2.112	-0.60943	7.32(-15)
0.02	2.012	-0.60366	—	0.06	2.198	-0.61285	1.49(-11)
0.03	2.031	-0.60497	—	0.065	2.28	-0.61501	3.94(-10)

beam fields in works [31–33] were based on conception of deformation of potential curves which results in coupling of the ground state $1s\sigma_g$ with $2p\sigma_u$ state [32]. This results in a possibility of rupture of the molecule after absorption some photons. On the other hand, the results obtained above enable us to analyse this process from simpler point of view. When the frequency of the radiation is low enough the consideration of the process as extension and rupture of the molecule in a strong static electric field is a quite adequate model [1,32]. The conception of coupling states might be substituted by an exact numerical calculation of one (as it was done above) or several (if several states are considered) dependencies $E(R)$. This numerical calculation is equivalent to a traditional calculation of the energy of the state when taking into account coupling with all the states of the same symmetry (corresponding to the symmetry of the initial physical problem).

The calculations presented above were carried out for the ground state of 2D Hamiltonian. In fact, our method is not restricted by these states. Computa-

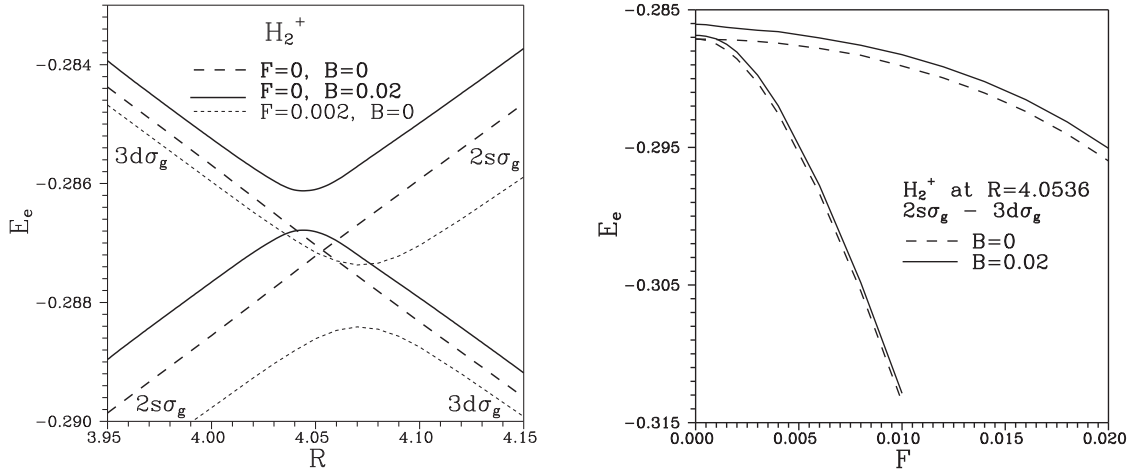


FIGURE 5. Left – The electron energies E_e of $2s\sigma_g$ and $3d\sigma_g$ states of the H_2^+ molecular ion as functions of the internuclear distance R in the field-free space (broken), in the magnetic field $\gamma = 0.02$ parallel to the molecular axis (full) and in the electric field $F = 0.002$ parallel to the molecular axis (dotted). Right – $E_e(F)$ for the doublet of $2s\sigma_g$ and $3d\sigma_g$ states of H_2^+ at $R = 4.0536$ a.u. for $\gamma = 0$ (broken) and $\gamma = 0.02$ (full).

TABLE 2. The ground state of the hydrogen atom in parallel electric and magnetic fields at $F = 0.1, 1, 5$.

	$F = 0.1$		$F = 1$		$F = 5$	
γ	E_0	$\Gamma/2$	E_0	$\Gamma/2$	E_0	$\Gamma/2$
0	-0.5274183	7.26904(-3)	-0.6243366	0.6468208	-0.1350071	3.083929
0.01	-0.532390	7.2624(-3)	-0.629329	0.646812	-0.140005	3.083925
0.1	-0.574600	6.6392(-3)	-0.673584	0.646053	-0.184739	3.083589
1	-0.8443098	9.5923(-5)	-1.0421379	0.577291	-0.6077008	3.050207
10	-1.7498730	—	-1.9579187	0.1173924	-2.375552	1.955678
100	-3.790110	—	-3.8219215	4.9988(-5)	-4.3806709	0.4909467
1000	-7.66247	—	-7.66807	—	-7.82561	1.04701(-2)

tional algorithms of our program of atomic and molecular mesh calculations AT-MOLMESH are constructed so that calculations are being carried out for a state with prescribed spatial symmetry and with the electron energy nearest to the given initial approximation E_b . Thus, there is no difference between calculations for the ground and for excited states and calculations can be fulfilled for various states of the same spatial symmetry including even degenerate states (when applying some special technical methods). For instance, potential curves $2s\sigma_g$ and $3d\sigma_g$ of the field-free H_2^+ have exact crossing near $R = 4.05$ [30]. In magnetic fields parallel to the molecular axis this pair of states forms an avoided crossing. Our method permits calculations for both exact and avoided crossings at $F = 0$ as well as at $F \neq 0$ as presented in Figure 5.

The second singe-electron system which we present here is the hydrogen atom in parallel electric and magnetic fields [23]. Some numbers obtained for this system are shown in Table 2.

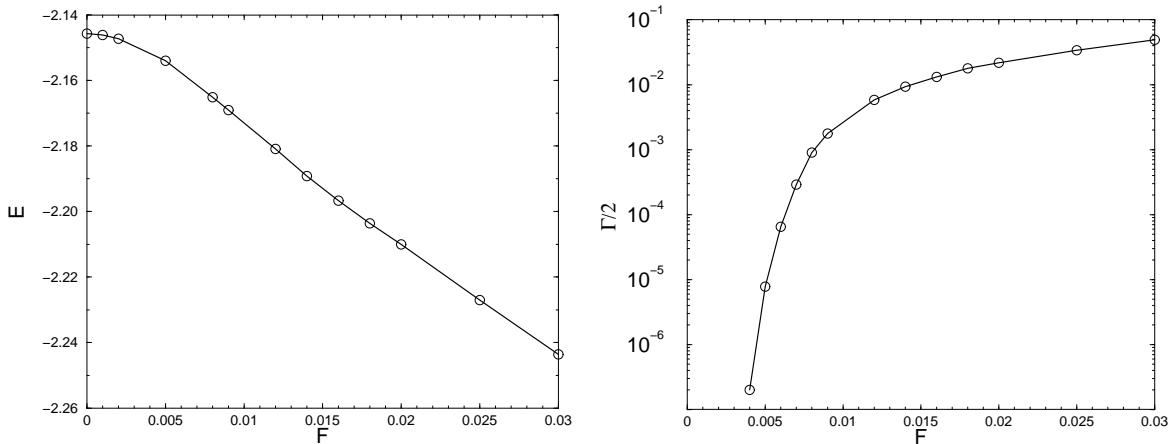


FIGURE 6. Left – The total energies of 2^1S_0 state of the helium atom dependent on the electric field strength. Right – Half-widths of this energy level.

Concluding this section we announce some preliminary results on the helium atom in strong electric fields. These results are obtained in a multi-configurational (CI) mesh calculation. The calculations for separate meshes are analogous to described above and are carried out by means of the curved path exterior complex transformation. Our preliminary results for the ground state of the helium atom agree with data from recent works [34,35]. Our results for the excited state 2^1S_0 are shown in Figure 6.

V CONCLUSIONS

In this communication we have presented a 2D fully numerical mesh solution approach to calculations for atoms and simple diatomic molecules in strong external electric and magnetic fields. For single-electron systems in external electric fields we can apply three different methods of calculation of the complex energy eigenvalues for atom-like systems and two methods for molecules. These methods have different but overlapping regions of their most effective application. This allows their combined using for the reciprocal control in applications. The complex boundary condition method is the most straightforward and is the most reliable in this sense. For relatively weak fields it allows obtaining results on the meshes with the lesser number of nodes than the curved path complex transformation. On the other hand, the boundary condition method loses its precision and stability at extremely strong electric fields and, second, this method contain the energy of the electron in its formulation. The latter feature can be some obstacle in its application to problems more complicated than the single-electron Schrödinger equation. The curved path complex transformation method is the most general of the three and the most prospective for the following applications. The only shortage of this method is that this is less precise and less stable for the atom-like systems at extremely strong electric fields ($|\text{Im}E| \gg |\text{Re}E|$) than the traditional complex rotation. Thus, the latter method is the most convenient for atom-like systems at such extremely strong fields.

The mathematical technique developed for solving Schrödinger equations for quasi-steady states allowed us to obtain a series of results for the hydrogen atom in parallel electric and magnetic fields and for the H_2^+ ion in strong electric fields. The following applications of these methods are associated with the CI approach which is now in the process of development and testing on the problem of the helium atom in strong electric fields. We present preliminary results for the 2^1S_0 state of this atom.

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